科学与工程计算课程报告

基于 R 语言

黄湘云

中国矿业大学 (北京) 理学院

2015 年 12 月 28 日

目录

Lorenz 方程组

$$\begin{cases} \dfrac{dx}{dt} = \sigma(y - x) \\ \dfrac{dy}{dt} = \rho x - y - xz \\ \dfrac{dz}{dt} = xy - \beta z \end{cases} \tag{1}$$

参数

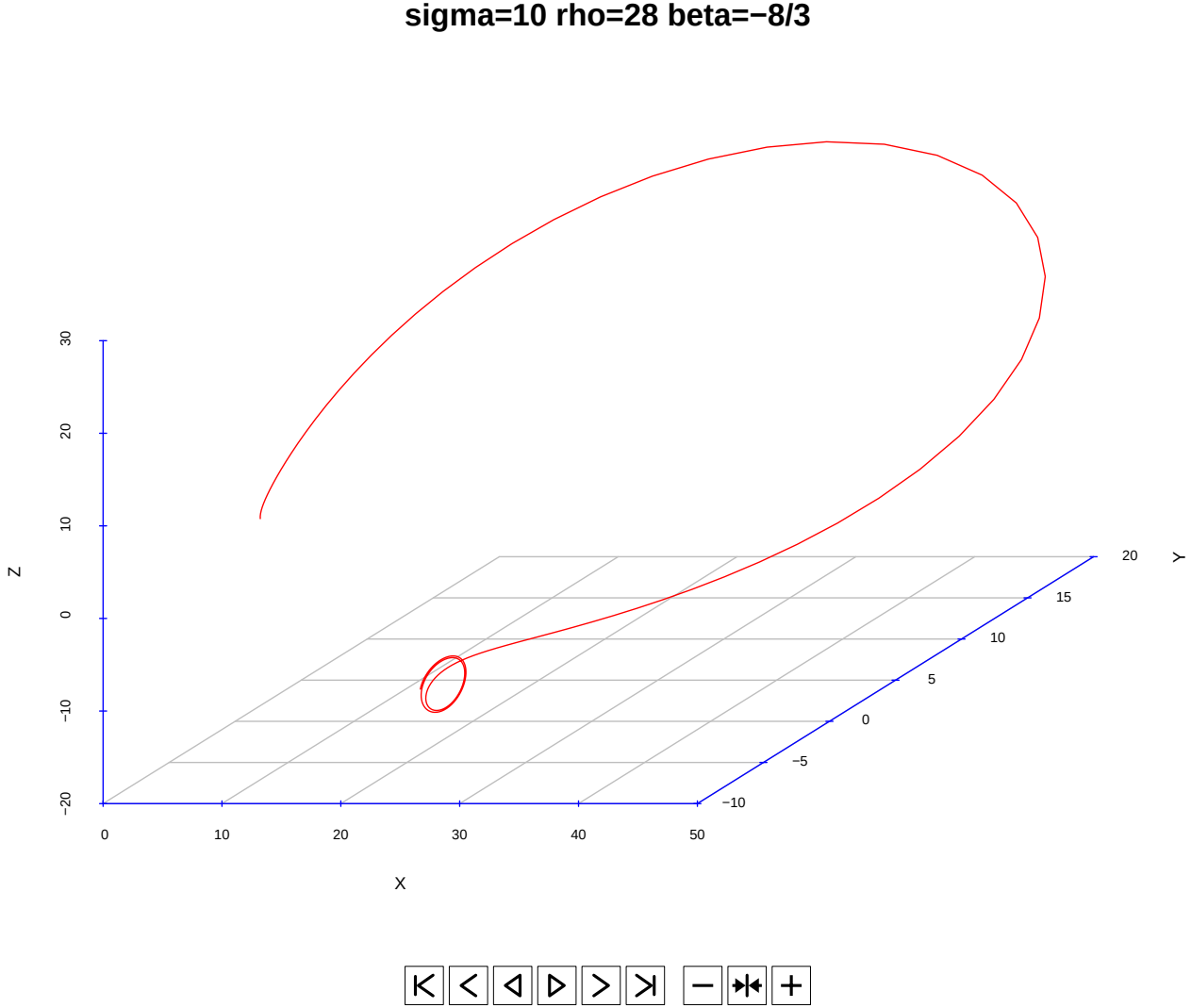
$$\sigma = 10, \rho = 28, \beta = \frac{8}{3}$$

初始条件

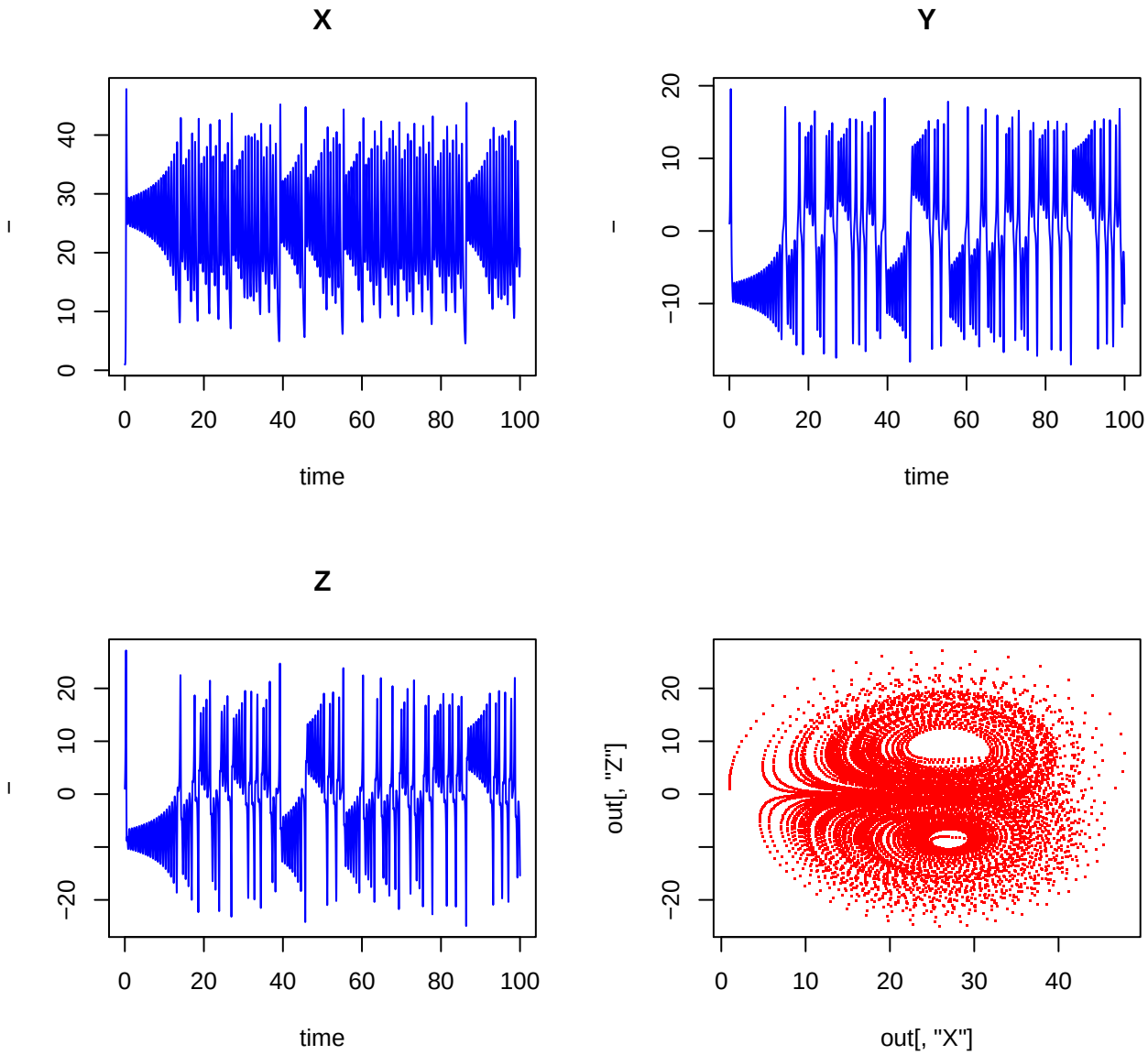
$$x(0) = y(0) = z(0) = 1$$

Lorenz 方程组

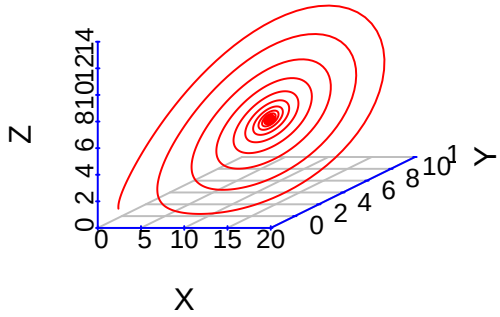
```
library(deSolve)
library(bvpSolve)
parameters <- c(a = -8/3,b = -10,c =  28)
state <- c(X = 1,Y = 1,Z = 1)
times <- seq(0, 100, by = 0.01)
Lorenz<-function(t, state, parameters) {
  with(as.list(c(state, parameters)),{
    dX <- a*X + Y*Z
    dY <- b * (Y-Z)
    dZ <- -X*Y + c*Y - Z
    list(c(dX, dY, dZ))
  })
}
out <- ode(y = state, times = times,
           func = Lorenz, parms = parameters)
```


sigma=10 rho=28 beta=−8/3
Z
30
20
10
0
−10
−20
X
0
10
20
30
40
50
Y
20
15
10
5
0
−5
−10

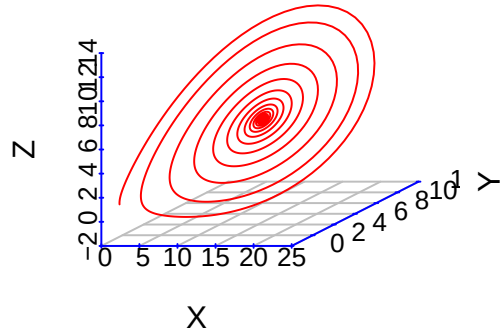
Lorenz model



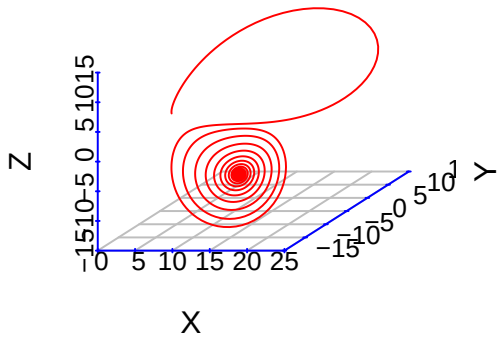
(−8/3,−10,13)



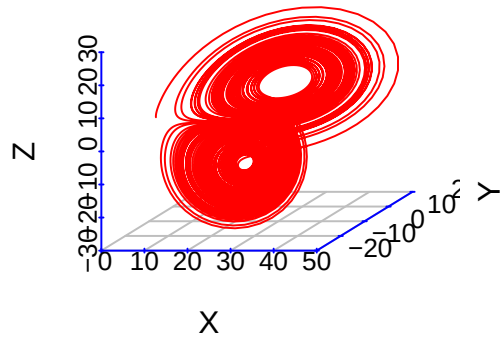
(−8/3,−10,14)



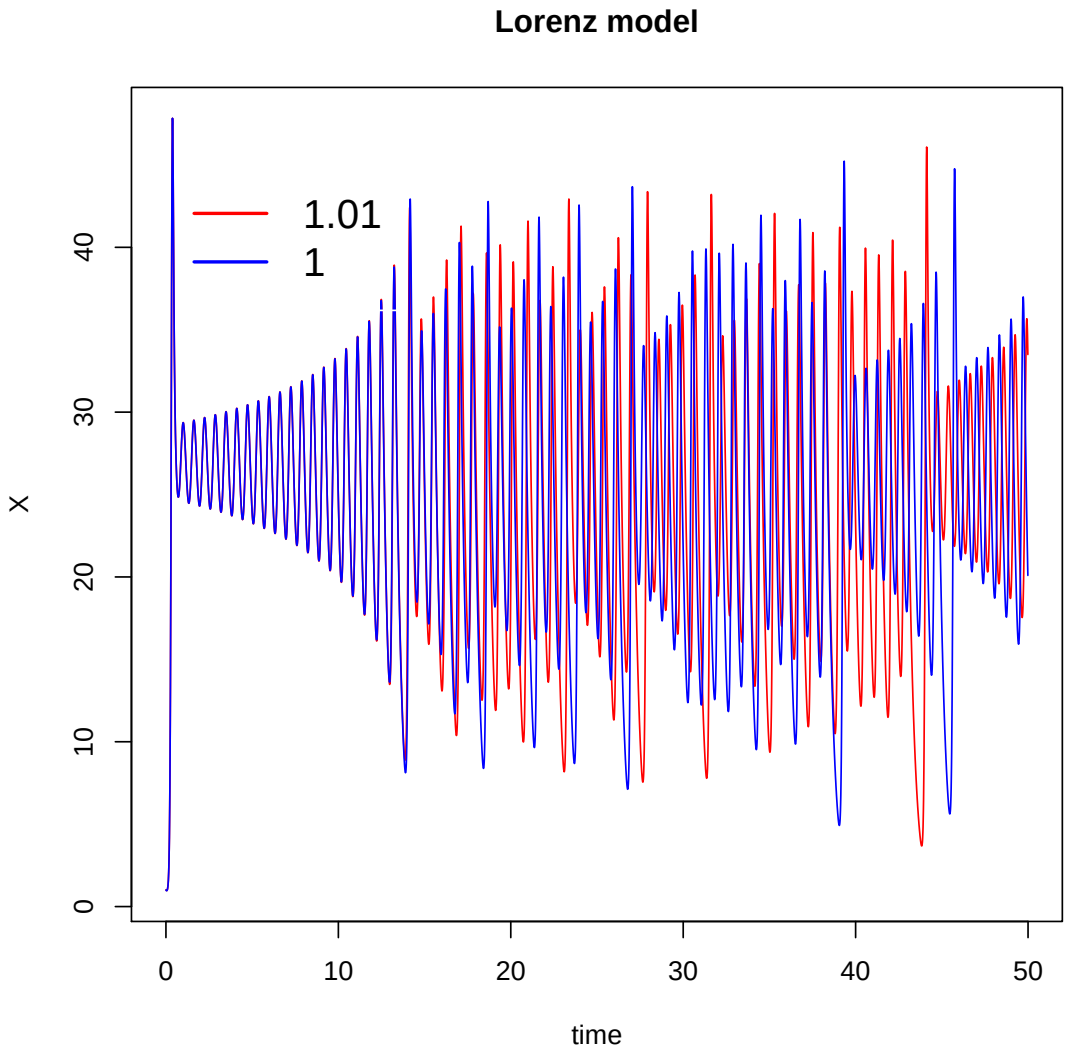
(−8/3,−10,15)



(−8/3,−10,28)



“蝴蝶”效应



求解器的性能表现

```
print(system.time(out  <- rk4   (state, times, Lorenz, parameters)))

##    user  system elapsed
##    1.17    0.00    1.17

print(system.time(out  <- lsode (state, times, Lorenz, parameters)))

##    user  system elapsed
##    0.42    0.00    0.43

print(system.time(out  <- lsoda (state, times, Lorenz, parameters)))

##    user  system elapsed
##    0.60    0.00    0.59
```

求解器的性能表现

```
print(system.time(out  <- lsodes(state, times, Lorenz, parameters)))

##    user  system elapsed
##    0.39    0.00    0.39

print(system.time(out  <- daspk (state, times, Lorenz, parameters)))

##    user  system elapsed
##    0.58    0.00    0.58

print(system.time(out  <- vode  (state, times, Lorenz, parameters)))

##    user  system elapsed
##    0.38    0.00    0.37
```

两点边值问题

$$\begin{cases} \epsilon \dfrac{d^2y}{dx^2} + \dfrac{dy}{dx} = a,\ 0 < a < 1 \\ y(0) = 0, y(1) = 1 \end{cases} \tag{2}$$

方程精确解

$$y = \frac{1-a}{1-e^{-\frac{1}{\epsilon}}}(1 - e^{-\frac{x}{\epsilon}}) + ax \tag{3}$$

为了把微分方程 (1) 离散，将 [0,1] 区间 n 等分，令 $h = 1/n$,

$$x_i = ih, i = 1, 2, ..., n-1 \tag{4}$$

得到差分方程

$$\epsilon \frac{y_{i-1} - 2y_i + y_{i+1}}{h^2} + \frac{y_{i+1} - y_i}{h} = a \tag{5}$$

两点边值问题

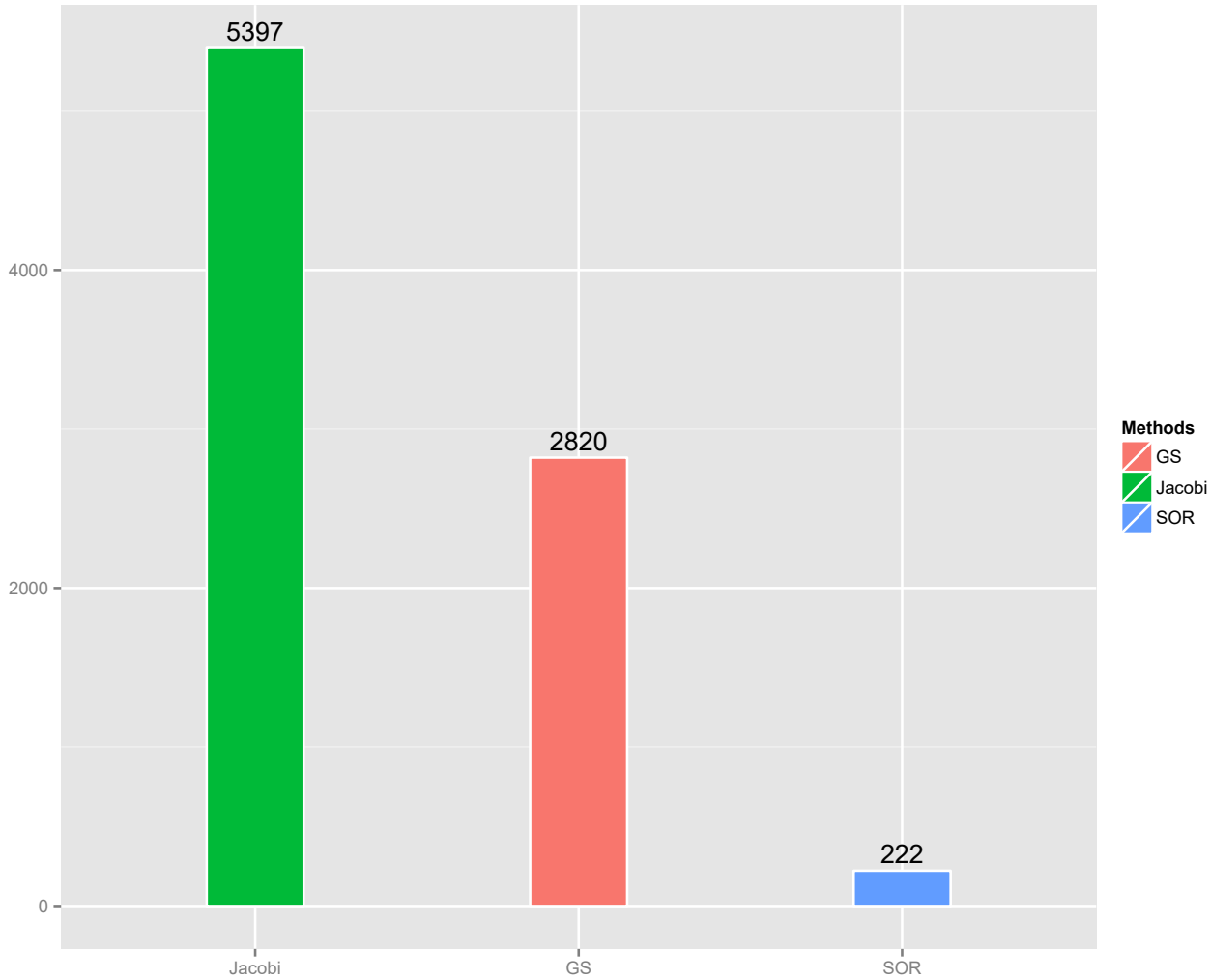
将方程 (4) 化简为

$$(\epsilon + h)y_{i+1} - (2\epsilon + h)y_i + \epsilon y_{i-1} = ah^2 \tag{6}$$

```
A[1:5,1:5]

##       [,1]  [,2]  [,3]  [,4]  [,5]
## [1,] -0.21  0.11  0.00  0.00  0.00
## [2,]  0.10 -0.21  0.11  0.00  0.00
## [3,]  0.00  0.10 -0.21  0.11  0.00
## [4,]  0.00  0.00  0.10 -0.21  0.11
## [5,]  0.00  0.00  0.00  0.10 -0.21
```

迭代次数

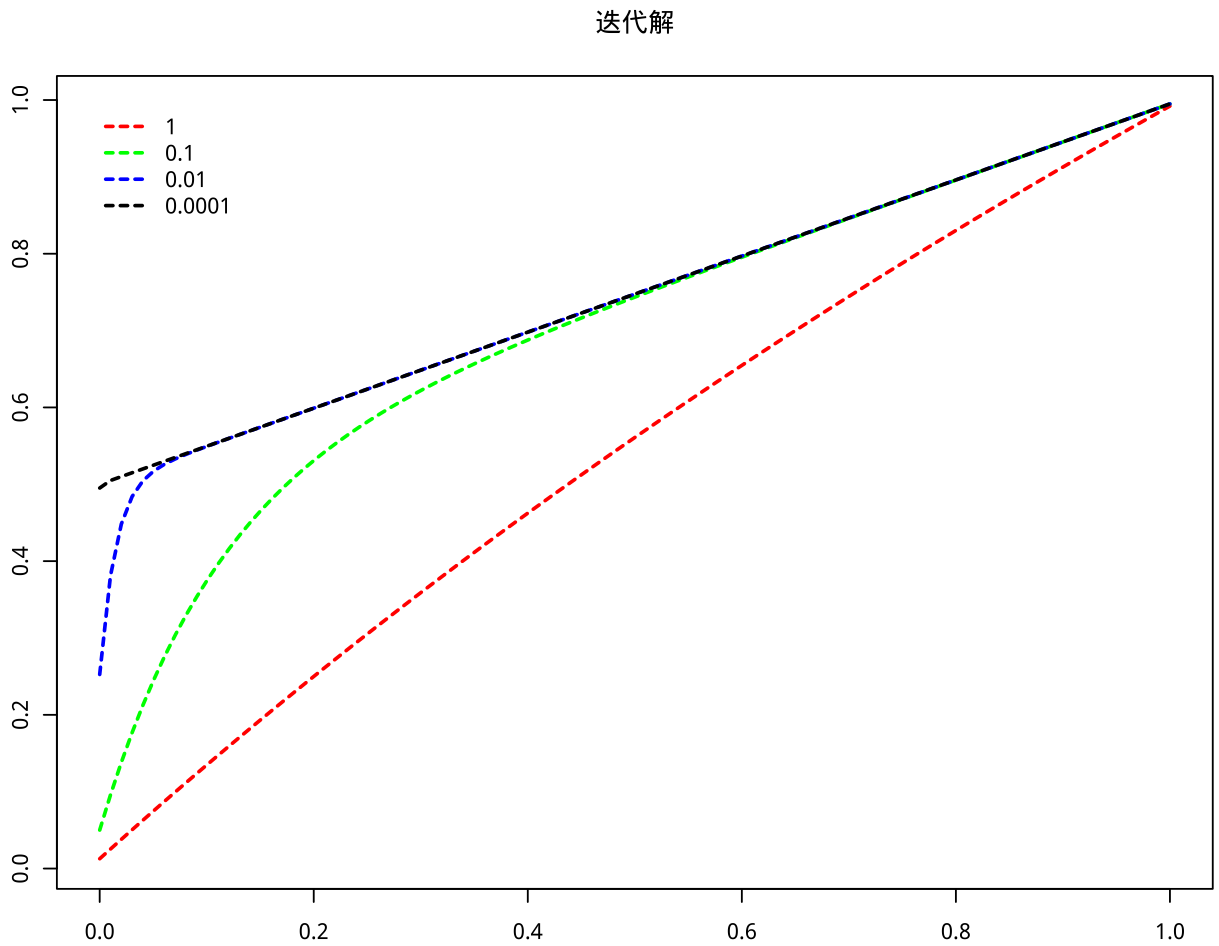


SOR 最佳松弛因子

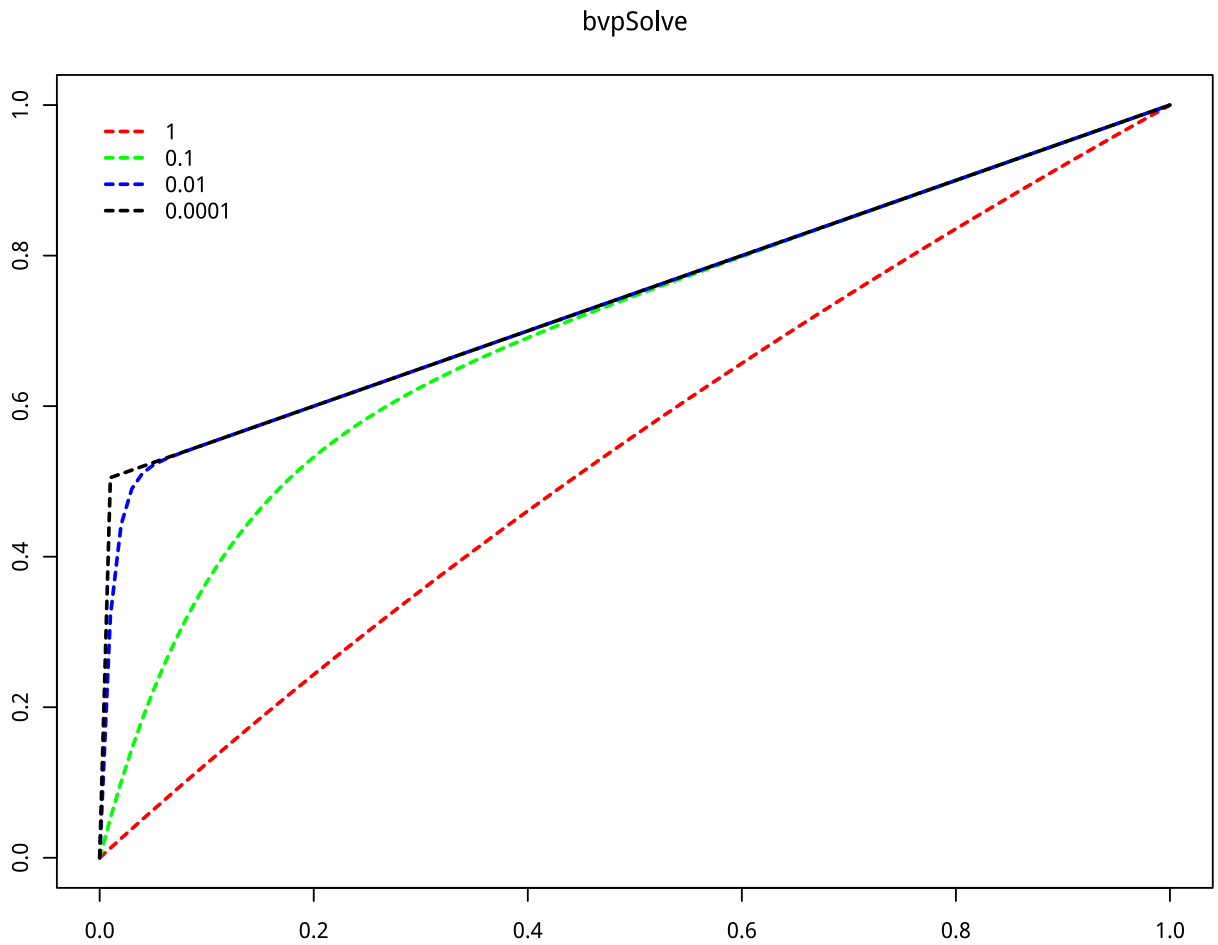
```
w <- seq(0,2,length.out = 200); e <- c(1,0.1,0.01,0.0001)
SOR_W <- rep(0,200);nmax=1000; iter_num <- matrix(rep(0),200,4)
for(i in seq(length(e))){
  A<-CoefMatrix(e=e[i],h=1/n,n)
  b<-VecB(a=1/2,h=1/n,e=e[i],n)
  for(j in seq(200)){
    solution_SOR<-SOR(A=A,b=b,x0=x0,w=w[j],nmax=nmax,eps=eps)
    iter_num[j,i]<-solution_SOR$iter_num
    SOR_W[j]<-solution_SOR$iter_err[500] } }
Pivot<-function(x){return(  which(x==min(x))[1] ) }
apply(iter_num[-1,],2,Pivot)

[1] 193 188 150 100
```

迭代法

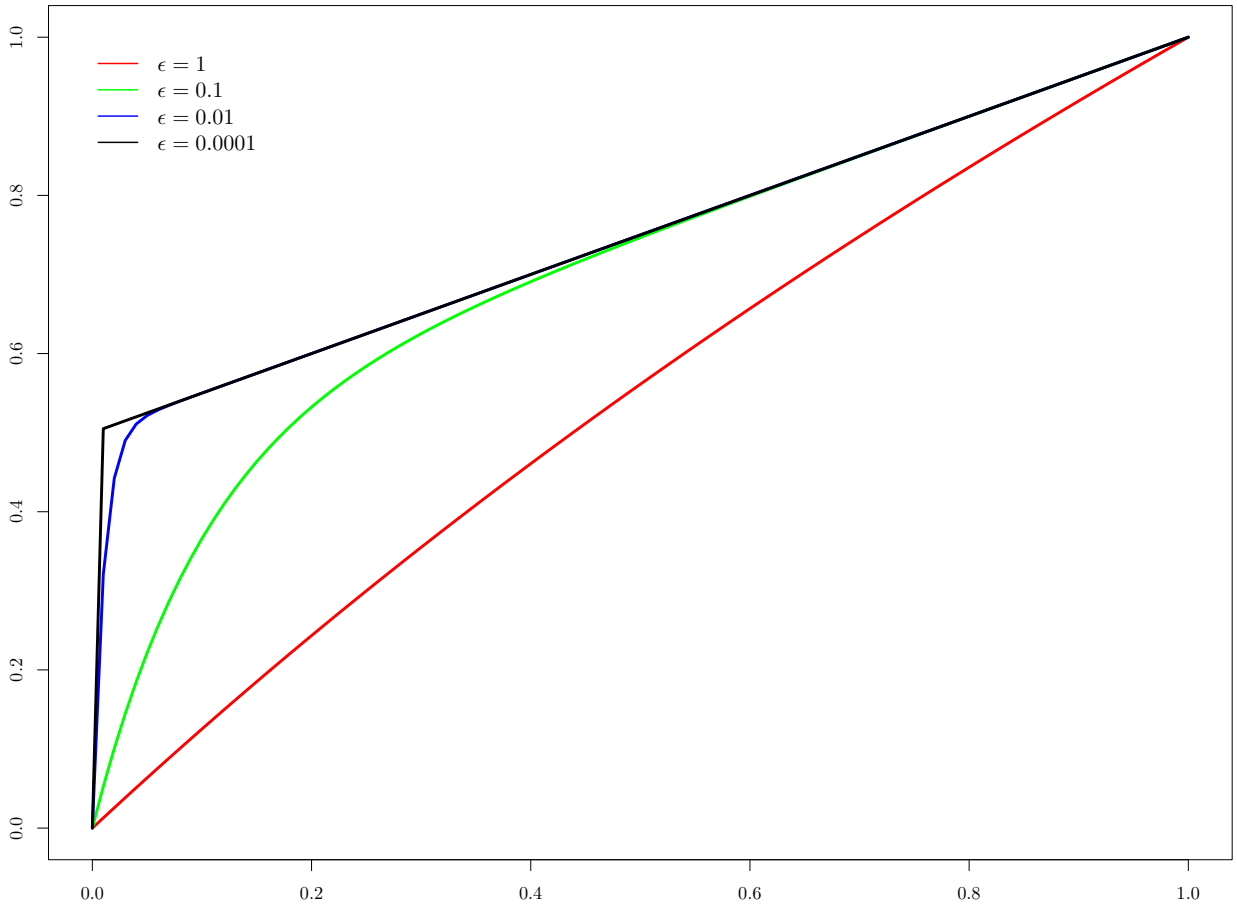


打靶法



解析解

$$f(x) = \frac{1-a}{1-e^{-\frac{1}{\epsilon}}}(1 - e^{-\frac{x}{\epsilon}}) + ax$$



一维热传导方程

$$\begin{cases} \frac{\partial y}{\partial t} = D\frac{\partial^2 y}{\partial x^2} \end{cases} \tag{7}$$

参数

$$D = 0.01$$

边界条件

$$y_{t,x=0} = 0, y_{t,x=1} = 1$$

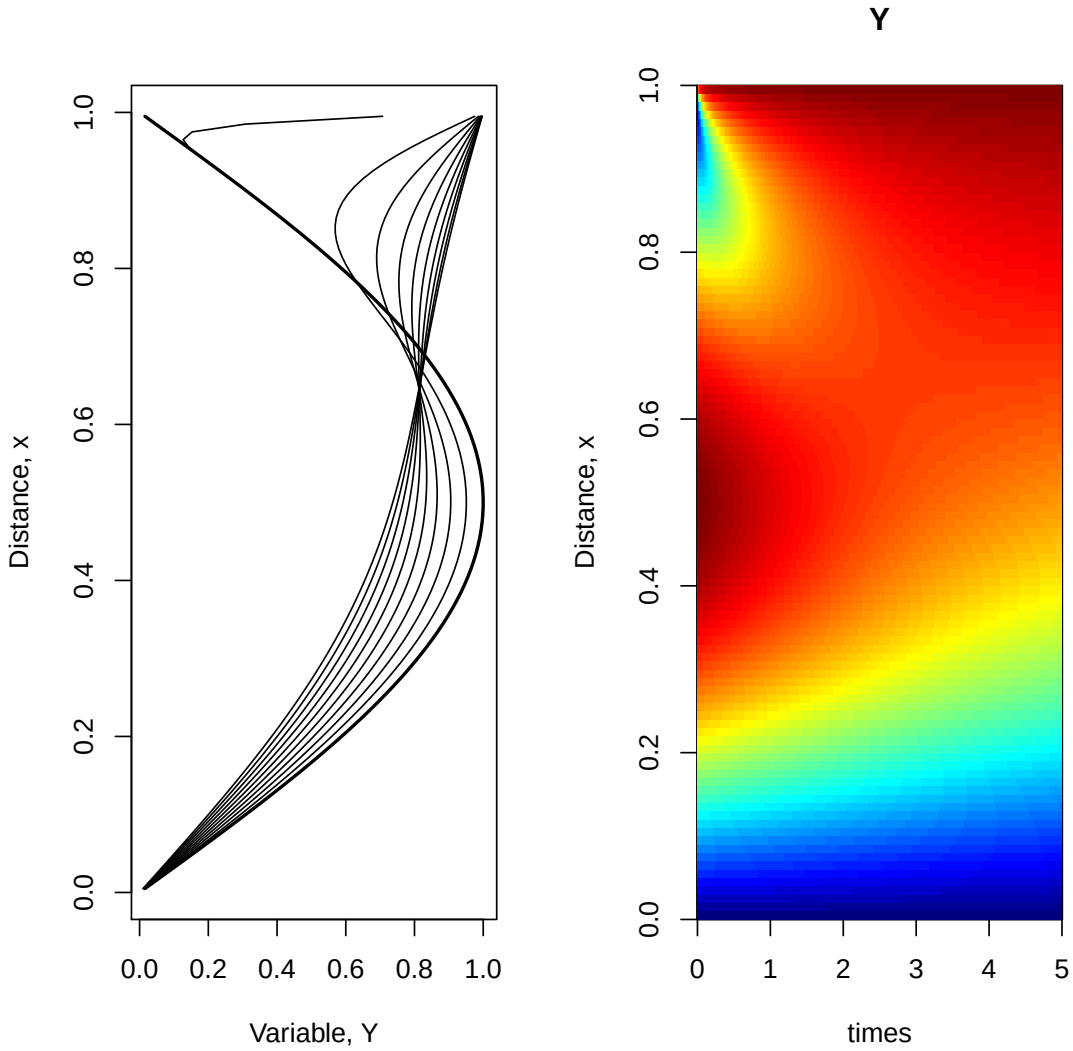
初始条件

$$y_{t=0,x} = sin(\pi x)$$

一维热传导方程

```
rm(list = ls())
library(ReacTran)
N <- 100
xgrid <- setup.grid.1D(x.up = 0, x.down = 1, N = N)
x <- xgrid$x.mid
D.coeff <- 0.01
Diffusion <- function (t, Y, parms){
  tran <- tran.1D(C = Y, C.up = 0, C.down = 1,
                  D = D.coeff, dx = xgrid)
  list(dY = tran$dC, flux.up = tran$flux.up,
       flux.down = tran$flux.down) }
Yini <- sin(pi * x)
times <- seq(from = 0, to = 5, by = 0.01)
out <- ode.1D(y = Yini, times = times, func = Diffusion,
                parms = NULL, dimens = N)
```

一维热传导方程


Y
Distance, x
0.0
0.2
0.4
0.6
0.8
1.0
Variable, Y
0.0
0.2
0.4
0.6
0.8
1.0
Distance, x
0
1
2
3
4
5
times

二维拉普拉斯方程

$$\begin{cases} \dfrac{\partial^2 u}{\partial x^2} + \dfrac{\partial^2 u}{\partial y^2} = 0 \end{cases} \tag{8}$$

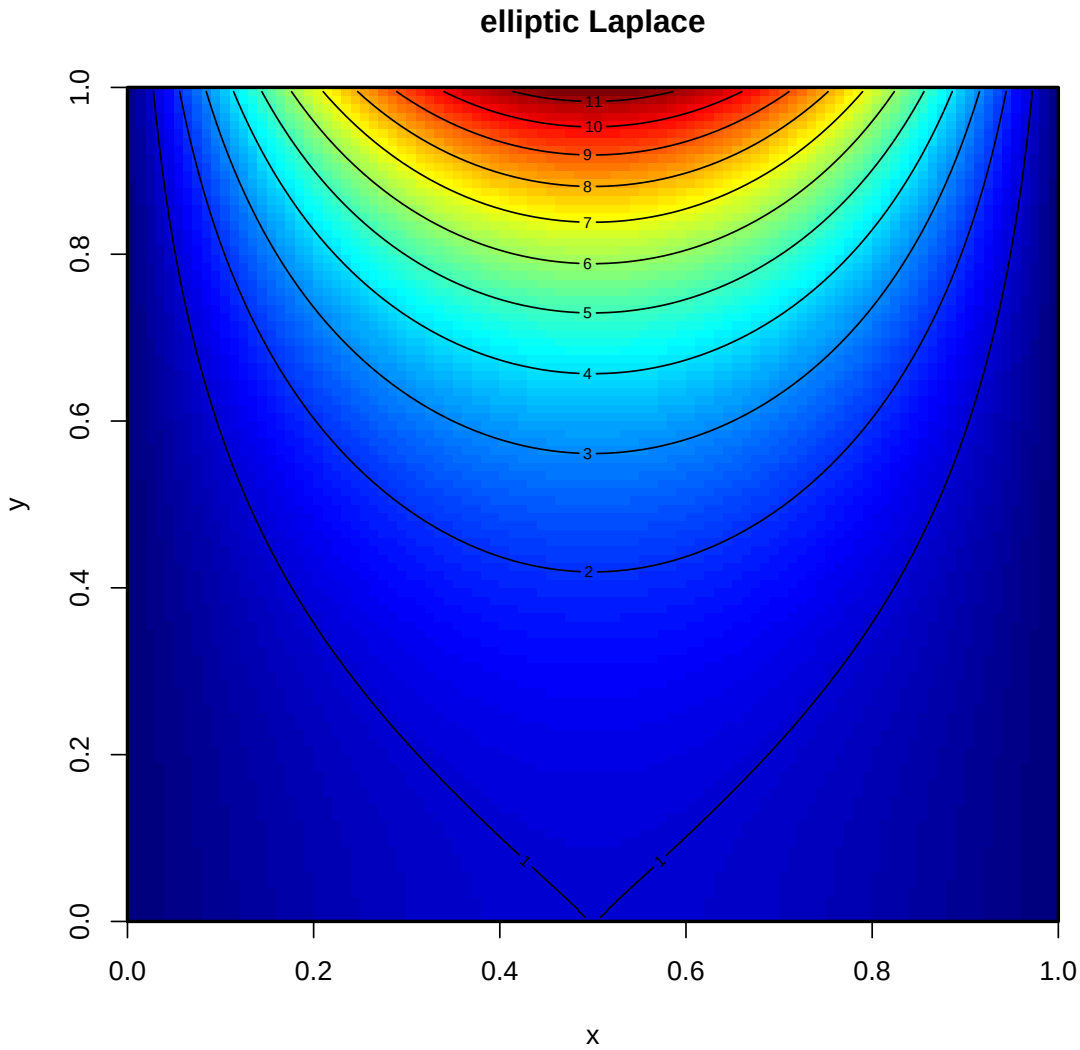
边界条件

$$\begin{cases} u_{x=0,y} = u_{x=1,y} = 0 \\ \dfrac{\partial u_{x,y=0}}{\partial y} = 0 \\ \dfrac{\partial u_{x,y=1}}{\partial y} = sin(\pi x)\pi sinh(\pi) \end{cases} \tag{9}$$

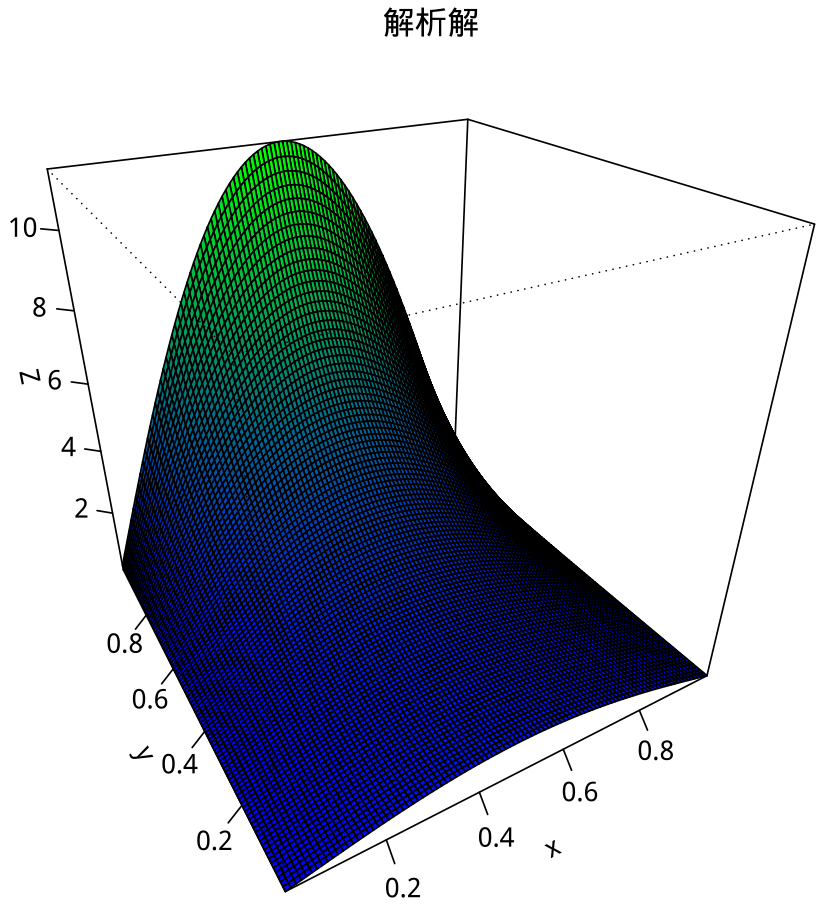
解析解

$$u(x, y) = sin(\pi x)cosh(\pi y)$$

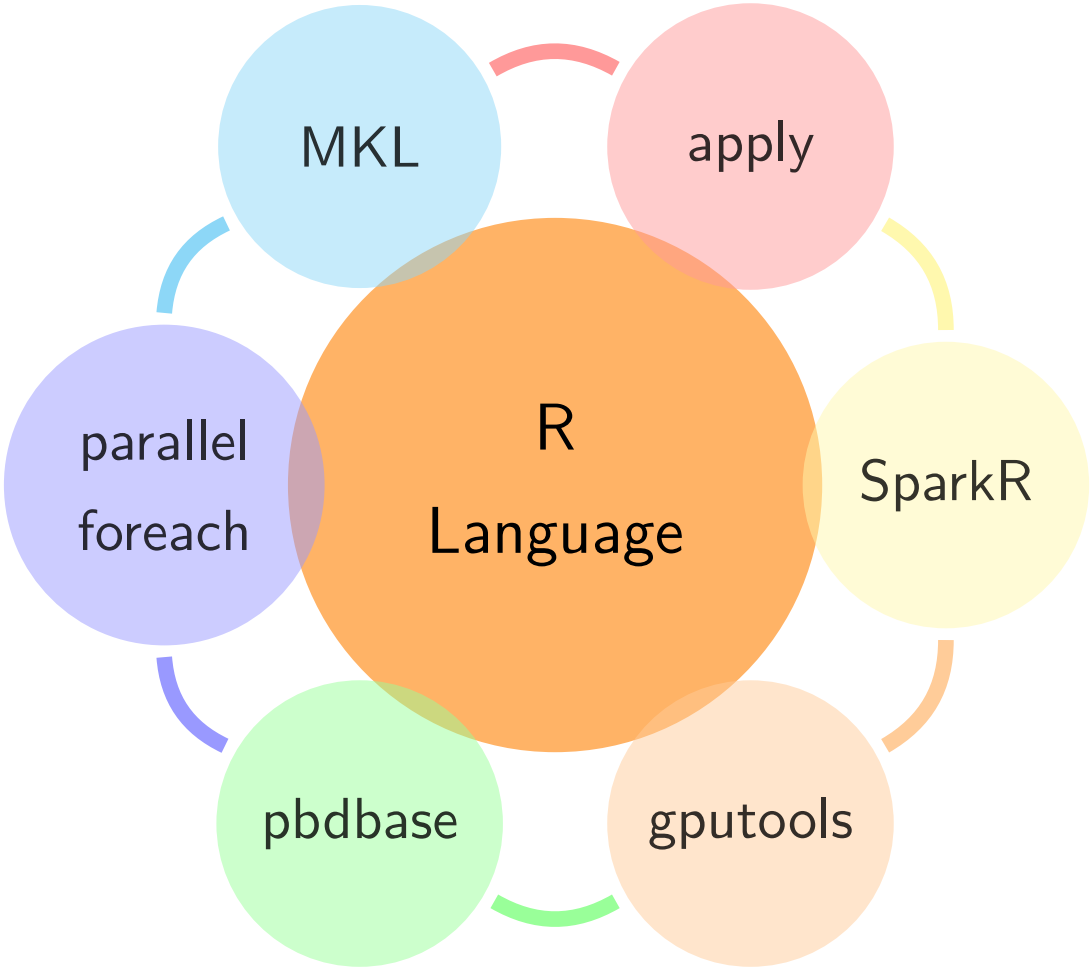
二维拉普拉斯方程



二维拉普拉斯方程



并行计算


MKL
apply
parallel
foreach
R
Language
SparkR
pbdbase
gputools

Revolution R Open 并行效果

	user	system	elapsed
8 核	0.01	0.02	7.56
6 核	0.02	0.01	8.14
4 核	0.01	0.02	9.50
2 核	0.00	0.01	15.06
单核	17.41	0.00	17.41

并行效果

	RRO	GotoBLAS	IntelMKL	R3.1.3	R3.2.3	Atlas
1	7.70	8.36	10.99	7.73	7.47	7.03
2	7.62	8.33	9.83	7.68	7.31	6.93
3	7.66	8.17	10.09	7.75	7.33	6.96

R is a free software environment for statistical computing and graphics.

```
               -
platform       x86_64-w64-mingw32
arch           x86_64
os             mingw32
system         x86_64, mingw32
status
major          3
minor          1.3
year           2015
month          03
day            09
svn rev        67962
language       R
version.string R version 3.1.3 (2015-03-09)
nickname       Smooth Sidewalk
```

R 扩展包

```
package      * version date       source
bvpSolve     * 1.2.4   2013-08-15 CRAN (R 3.1.2)
deSolve      * 1.11    2014-10-29 CRAN (R 3.1.2)
devtools       1.6.1   2014-10-07 CRAN (R 3.1.2)
evaluate       0.8     2015-09-18 CRAN (R 3.1.3)
formatR        1.2.1   2015-09-18 CRAN (R 3.1.3)
highr          0.5.1   2015-09-18 CRAN (R 3.1.3)
knitr        * 1.11    2015-08-14 CRAN (R 3.1.3)
magrittr       1.5     2014-11-22 CRAN (R 3.1.3)
RColorBrewer * 1.1.2   2014-12-07 CRAN (R 3.1.3)
ReacTran     * 1.4.2   2014-12-26 CRAN (R 3.1.3)
```

R 扩展包

```
package       * version date       source
rootSolve     * 1.6.5.1 2014-11-06 CRAN (R 3.1.2)
rstudioapi      0.4.0   2015-12-09 CRAN (R 3.1.3)
scatterplot3d * 0.3.36  2015-07-30 CRAN (R 3.1.3)
shape         * 1.4.2   2014-11-05 CRAN (R 3.1.2)
showtext        0.4.4   2015-10-30 CRAN (R 3.1.3)
showtextdb      1.0     2015-03-10 CRAN (R 3.1.3)
stringi         0.4.1   2014-12-14 CRAN (R 3.1.3)
stringr         1.0.0   2015-04-30 CRAN (R 3.1.3)
sysfonts        0.5     2015-04-27 CRAN (R 3.1.3)
```

Thank you!

黄湘云

Email: xiangyunfaith@outlook.com

Q & A

参考文献

Karline Soetaert, Thomas Petzoldt, R. Woodrow Setzer (2010)

Solving Differential Equations in R: Package deSolve

Journal of Statistical Software 33(9), 1 – 25.

Ligges, U. and Machler, M. (2003)

Scatterplot3d – an R Package for Visualizing Multivariate Data

Journal of Statistical Software 8(11), 1 – 20.

Karline Soetaert, Jeff Cash and Francesca Mazzia (2013)

bvpSolve: Solvers for boundary value problems of ordinary differential equations

R package version 1.2.4 http://CRAN.R-project.org/package=bvpSolve.

Charlie Sharpsteen and Cameron Bracken (2015)

tikzDevice: R Graphics Output in LaTeX Format

R package version 0.8.1 http://CRAN.R-project.org/package=tikzDevice.

参考文献

Yihui Xie (2013)

animation: An R Package for Creating Animations and Demonstrating Statistical Methods

Journal of Statistical Software 53(1), 1-27.

R Core Team (2015)

R: A language and environment for statistical computing.

R Foundation for Statistical Computing https://www.R-project.org/.

Soetaert, Karline and Meysman, Filip (2012)

Reactive transport in aquatic ecosystems: Rapid model prototyping in the open source software R

Environmental Modelling & Software 32(3), 49-60.